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13. ABSTRACT *(Maximum 200 words)*
This DURIP-funded Beowulf cluster will enhance our AFOSR-funded research in several areas. Large-scale modeling of complex systems in the areas of corroision and catalysis is a vital Air Force need. Our previous computational resources alone would not allow us to pursue the most important and complex portions of our currrent contact with AFOSR. The DURIP funding has now provided our personnel with the computational capability to examine the corrosion of aluminum alloys, to understand the role of stress fields in materials and in the multi-scale modeling of fatigue and fracture, and to study reactivity on patterned surfaces including superlattice, nanoparticles, and piezoelectric oxide supported metal. To perform this research, we will use ab-initio density functional theory (DFT), which gives quantitative results by detailed modeling of the valence electrons in materials. The DFT has repportedly proven itself as a highly accurate and highly efficient first-principles compuational tool. However, since DFT is a quantum-mechanical method, high accuracy on real-world systems requries significant computational cost. This grant, by funding a Beowulf cluster supercomputing environment, has provided a novel computer architecture which will enable AFOSR-funded researchers to gain new insights into materials of Air Force needs.

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Beowulf Cluster for Computational Corrosion and Catalysis Studies
Award No. F49620–01–1–0345
Final Performance Report

Andrew M. Rappe

August 11, 2002

Identification of Acquired Equipment

The granted funds were expended for the purchase of a Beowulf cluster from Aspen Systems. The system includes one front-end node, with monitoring console and LCD screen, and 63 compute nodes. Each of the 63 nodes contains two 1.7 GHz Pentium 4 CPUs, 1 or 2 GB of RDRAM memory, and 18 GB of SCSI hard disk space. Power supplies, tower racks, ethernet cables, and switches were included to enable the nodes to function as a single Beowulf cluster supercomputer. A complete list of parts is included as an additional attachment (`UPennScope.pdf`).

The attachment shows a price quotation of $226,000. However, due to delays in delivery by Aspen Systems and other problems, the company reduced the price by 3%, making the final price $219,220. An additional $780 was spent on important spare parts for the cluster, bringing the total expense to the $220,000 awarded.

The Beowulf cluster was ordered in fall 2001, and it was received by the University of Pennsylvania in January 2002. After burn-in and testing by the research group at Penn and reconfiguration by Aspen Systems personnel, payment for the cluster was released in February 2002. Thus, the entire transaction was concluded during the Period of Performance.

Summary of Research Project

This DURIP-funded Beowulf cluster will enhance our AFOSR-funded research in several areas. Large-scale modeling of complex systems in the areas of corrosion and catalysis is a vital Air Force need. Our previous computational resources alone would not allow us to pursue the most important and complex portions of our current contract with the AFOSR. The DURIP funding has now provided our personnel with the computational capability to

examine the corrosion of aluminum alloys, to understand the role of stress fields in materials and in the multi-scale modeling of fatigue and fracture, and to study reactivity on patterned surfaces including superlattices, nanoparticles, and piezoelectric oxide supported metals. To perform this research, we will use *ab-initio* density functional theory (DFT), which gives quantitative results by detailed modeling of the valence electrons in materials. DFT has repeatedly proven itself as a highly accurate and highly efficient first-principles computational tool. However, since DFT is a quantum-mechanical method, high accuracy on real-world systems requires significant computational cost. This grant, by funding a Beowulf cluster supercomputing environment, has provided a novel computer architecture which will enable AFOSR-funded researchers to gain new insights into materials of Air Force need.